

MM 20: Electronic Properties II

Time: Tuesday 10:15–11:30

Location: H 0111

MM 20.1 Tue 10:15 H 0111

Non local exchange and correlations in Fe — ●GERNOT STOLLHOFF — MPI f. Festkörperforschung, Heisenbergstr.1, D 70569 Stuttgart

Density functional (DF) calculations obtain the correct ferromagnetic ground state of Fe. We had in the past demonstrated with the help of correlation calculations on 5 band Hubbard Hamiltonians that this is in part due to a chance compensation of big errors in the handling of local interactions. DMFT-calculations on similar models have shown that the biggest apparent DF-deficiency, the computed transition temperature, can be only partially improved, namely from 3500K to 2000K.

Recent ab-initio correlation calculations by the Local Ansatz falsify the underlying rigid band hypothesis in both approaches. While the non magnetic DF-results are the appropriate basis for the magnetic ground state, they fail for the non magnetic state itself. Here, not fully screened non local exchange contributions play a big role. The exact charge distribution is different, and the density of state is strongly modified, with $n(E_F)$ less than half the one of the DF-case. This causes an electronic first order phase transition. Also the resulting energy-bands differ. In contrast to the DF-results, these explain temperature dependent angular resolved photoemission experiments (Kirschner et al., PRL 53, 612 (1984)).

MM 20.2 Tue 10:30 H 0111

Transport through realistic junctions: Beyond DFT — ●FRANK FREIMUTH¹, DANIEL WORTMANN¹, YURIY MOKROUSOV², and STEFAN BLÜGEL¹ — ¹Institut für Festkörperforschung, Forschungszentrum Jülich, Germany — ²Institut für Angewandte Physik, Universität Hamburg

DFT-based *ab initio* methods have become the standard tools for the investigation of materials' properties. However, the applicability of this method to electronic transport calculations is limited by the difficulties of describing excited states by ground state DFT. In this talk, we give an outline of how the local part of the Coulomb interaction may be taken into account via the self-energy in calculations describing electronic transport. Wannier functions constructed from the DFT Bloch states of the interface provide a localized set of basis functions adequate for the calculation of correlation effects using many-body techniques formulated for lattice systems. Our electronic transport method is based on the embedding technique, which provides a tool to calculate the Green function of the interface region of planar junctions suitable for application within *ab initio* studies of electronic transport. Our implementation of the embedding technique uses the full-potential linearized augmented plane-wave (FLAPW) method which does not make any approximations to the potential.

MM 20.3 Tue 10:45 H 0111

Fermiology of Cuprates and Non-Fermi Liquid Metallic Phases. — ●MUKUL LAAD, LIVIU HOZOI, and PETER FULDE — Max-Planck Institut fuer Physik komplexer Systeme, 38 Noethnitzer Strasse, 01187 Dresden, Germany

In the first step, we employ ab-initio wave-function based quantum chemical calculations to extract the effective hoppings for one hole/electron doped into a CuO₂ plane. Strong, anisotropic, short-range spin correlations are found to drastically modify (bare) density-functional estimates of the hoppings. Remarkably, our results describe the detailed dispersion of the Zhang-Rice-like band (hole doping) as well as the unique evolution of both, hole- and electron-doped cuprates with quantitative accuracy. We discuss the implications of our findings for many, Fermi surface based, physical responses and their evolution in cuprates as a function of doping.

In the second step, we build upon these results to study the dynamical correlations in cuprates by incorporating these results in a new cluster dynamical mean field approximation. The physical mechanisms underlying the emergence of the unique non-Fermi liquid metallic phase(s) in cuprates will be detailed, and several response functions will be described in relation to experiments.

MM 20.4 Tue 11:00 H 0111

Quantum-chemical approach to cohesive properties of metals: Anomalous behaviour of Be. — ●ELENA VOLOSHINA¹, BEATE PAULUS², and HERMANN STOLL³ — ¹Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden — ²Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustraße 3, D-14195 Berlin — ³Institut für Theoretische Chemie, Universität Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart

Calculations based upon the incremental scheme [1], i.e. an expansion of the total correlation energy in terms of one-body, two-body and higher-order contributions, have been performed on a variety of solids with band gaps [2]. Metals require a special treatment. Via an embedding scheme, we can force localization in metallic-like model systems and can mimic the metallic band structure within finite fragments of the solid [3]. This allows for a gradual delocalization towards the infinite crystal within the incremental scheme. Up to now we successfully applied the method to magnesium [4] and group 12 elements [5,6] where in all cases the ground-state properties agree very well with experiment. The beryllium crystal has the same hcp structure as Mg; the atoms are characterized by closed ns^2 shells. At the same time Mg is almost free-electron-like whereas Be, although in general metallic, shows a lower density of states of almost entirely p character at the Fermi energy; that is the reason for the anomalous behavior of Be compared with other group 2 and 12 metals.

[1] PRB 46, 6700 (1992).

[2] Phys. Rep. 428, 1 (2006).

[3] JCP 126, 134115 (2006).

[4] PRB 75, 245117 (2007).

[5] PRB 74, 094102 (2006).

[6] PRB (in press).

MM 20.5 Tue 11:15 H 0111

Does magnesium-like zinc in a nearly ideal hcp form exist? — NICOLA GASTON¹, ●BEATE PAULUS², ULRICH WEDIG³, and MARTIN JANSEN³ — ¹Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden — ²Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin — ³Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

Zinc crystallises in the hcp structure, but with an anomalously large c/a ratio, indicating a strong distortion away from ideal packing. Density functional calculations of zinc fail to describe the unusual hcp structure of this material [1]. We perform a wavefunction-based correlation treatment on top of periodic Hartree-Fock calculations. This treatment corresponds to a many-body expansion of the correlation energy of the extended system in terms of localized orbital groups (method of increments)[2]. The Hartree-Fock treatment yields no binding and no equilibrium geometry for zinc. The binding of the ground-state structure is fully described by electronic correlations. Our values of the cohesive energy agree within 5% with the experimental value and within 2% for the lattice parameters. These calculations indicate additionally a local minimum of the potential energy surface for a c/a ratio which is almost ideally close-packed as in magnesium.

[1] B. Paulus, K. Rosciszewski, P. Sony, U. Wedig and M. Jansen Phys. Rev. B 75, 205123 (2007).

[2] N. Gaston and B. Paulus, Phys. Rev. B in press (2007)